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IMPROVED NUMERICAL MODELING OF GROUNDWATER FLOW AND TRANSPORT AT THE MADE-2 SITE

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Public domain computer programs were used to attempt an improved model of the tritium plume observed during Macrodispersion Experiment 2 (MADE-2), a field scale natural gradient experiment conducted at Columbus Air Force Base, Mississippi. A computational grid having 66 rows, 21 columns, and 9 layers was used. The finite difference program MODFLOW was used to simulate the flow of groundwater through a 330 m x 105 m computational domain. Solutions for the 468 day experiment were obtained using a Sun Sparcstation 2 for several choices of convergence and storage parameters. The simulations had small mass balance errors and were consistent with continuous head observations. The smallest storage coefficients gave the best agreement. The flow model is about as accurate as the data permit. Tritium plume simulations used the mixed Lagrangian-Eulerian finite difference program MT3D to solve the contaminant transport equation using the MODFLOW-predicted flow field. Thirteen runs were made using various advection algorithms and dispersivities, but none was successful. Numerical instabilities or grossly unrealistic predictions ended every run by simulation day 141. Further work is needed to obtain a satisfactory plume prediction.

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PREFACE

This report was originally prepared for RDL under Contract number F49620-93-C-0063 for the Air Force Office of Scientific Research, Bolling Air Force Base, Washington D.C. It contains results of summer faculty research sponsored by the Armstrong Laboratory Environics Directorate, Tyndall Air Force Base, Florida 32403-5323.

This report covers research performed by Dr. Donald D. Gray and Dale F. Rucker of West Virginia University between June and August 1994. The report is being reprinted and submitted to Defense Technical Information Center because of its widespread interest to the DOD regarding the fate and transport of hazardous wastes. The AL/EQC Mentor was Dr. Thomas B. Stauffer. Mary Reynolds was the AL/EQ Summer Faculty Coordinator.

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Abstract

Public domain computer programs were used to attempt an improved model of the tritium plume observed during Macrodispersion Experiment 2 (MADE-2), a field scale natural gradient experiment conducted at Columbus Air Force Base, Mississippi. The program Geo-EAS used head and hydraulic conductivity data at a relatively small number of irregularly spaced test locations to estimate corresponding values at the more numerous nodes of a computational grid having 66 rows, 21 columns, and 9 layers. The finite difference program MODFLOW was used to simulate the flow of groundwater through a 330 m x 105 m computational domain. The recent BCF2 subroutine package, which permits rewetting of cells, allowed the vertical discretization to be more accurate than in previous studies. Solutions for the 468 day experiment were obtained using a Sun Sparcstation 2 for several choices of convergence and storage parameters. The simulations had small mass balance errors and were consistent with continuous head observations. The smallest storage coefficients gave the best agreement. One persistent feature of the predicted head field was a tendency for the head to decline toward the northwest. This suggests that the plume should bend toward the northwest, but the observations show a bend toward the northeast. This discrepancy is probably due to inaccurate head boundary conditions resulting from a lack of piezometers in the northern part of the computational domain. The flow model is about as accurate as the data permit.

Tritium plume simulations used the mixed Lagrangian-Eulerian finite difference program MT3D to solve the contaminant transport equation using the MODFLOW-predicted flow field. Thirteen runs were made using various advection algorithms and dispersivities, but none was successful. Numerical instabilities or grossly unrealistic predictions ended every run by simulation day 141. Further work is needed to obtain a satisfactory plume prediction.

IMPROVED NUMERICAL MODELING OF GROUNDWATER FLOW AND TRANSPORT AT THE MADE-2 SITE

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INTRODUCTION

Faced with the need to remediate groundwater pollution at many of its bases, the Air Force has undertaken an extensive program of research on subsurface contaminant transport. The Macrodispersion Experiment 2 (MADE-2), conducted together with the Electric Power Research Institute and the Tennessee Valley Authority, was a key element of this effort. MADE-2 was a field-scale natural gradient experiment performed in 1990-91 at Columbus Air Force Base in Columbus, Mississippi. A MADE-2 database has been prepared by Boggs and others (1993a) and analyses have been published by Boggs and others (1993b) and by Stauffer and others (1994).

The MADE-2 test site was an area about 300 m x 200 m with about 2 m of relief. It was covered primarily by weeds and brush, and contained no streams or ponds. The 10 m to 15 m thick upper layer of soil was a shallow alluvial terrace containing an unconfined aquifer. This was bounded below by an aquitard of marine silt and clay (Boggs, Young, Benton, and Chung; 1990). The aquifer soil was classified as poorly sorted to well sorted sandy gravel and gravelly sand with minor amounts of silt and clay. The aquifer was found to consist of irregular lenses and layers having typical horizontal dimensions on the order of 8 m and typical vertical dimensions on the order of 1 m.

The heterogeneity of the MADE-2 site was much greater than that of other reported natural gradient macrodispersion experiments. Measurements using the borehole flowmeter method showed hydraulic conductivity variations of up to four orders of magnitude in individual profiles. Rehfelt, Boggs, and Gelhar (1992) found that the variance of the natural logarithm of the hydraulic conductivity was at least an order of magnitude larger at Columbus than at Borden, Twin Lakes, or Cape Cod. The horizontal and vertical correlation scales for hydraulic conductivity were also larger by factors of 1.75 or more.

MADE-2 focused on the fate and transport of dissolved organic chemicals of the types found in jet fuels and solvents. A volume of 9.7 m^3 of tracer solution was injected at a constant rate for 48.5 hours through 5 wells spaced 1 m apart. The

solution contained tritiated water (an essentially passive tracer), benzene, naphthalene, p-xylene, and o-dichlorobenzene. The spread of the plume in three dimensions was monitored for 15 months by analyzing water samples drawn from up to 328 multilevel sampling wells (at up to 30 depths per well) and 56 BarCad positive displacement samplers. Five comprehensive sets of water samples (called snapshots) were obtained at intervals of about 100 days. Plots of concentration contours in horizontal planes showed that the tritium plume spread in an essentially linear fashion with a tendency to bend toward the northeast. The vertical structure along the plume axis was complex.

Boggs and others (1993b), based on numerical integration of the tritium concentrations, found ratios of observed mass to injected mass in the first four snapshots of 1.52, 1.05, 0.98, and 0.77, respectively. The 52% overestimate in the initial snapshot was attributed to preferential sampling from more permeable zones and to vertical interconnections between sampling points. The 23% underestimate in snapshot 4 was partially due to the motion of the plume's leading edge past the farthest downstream sampling points. Snaphot 5 was not intended to define the entire plume.

Our objective in the 1994 Summer Research Program was to obtain improved simulations of the MADE-2 tritium plume using public domain computer codes for groundwater flow and contaminant transport. The present work is an extension of the senior author's previous efforts as an AFOSR Summer Faculty Fellow (Gray, 1992; 1993).

FLOW MODELING

In accord with most groundwater studies, in the present work the effects of density variations are assumed to be negligible, so that the flow equation can be solved without knowing the concentration field. The resulting velocity field is input to the transport equation, which is then solved for the concentrations. These calculations were performed using computer programs MODFLOW for the flow problem and MT3D for the transport problem. Many other programs were used to prepare input files or to analyze results. Unless noted otherwise, these were written by the authors of this report in FORTRAN 77.

MODFLOW (McDonald and Harbaugh, 1988) is a U. S. Geological Survey (USGS) public domain FORTRAN 77 program for the solution of the groundwater flow equation. The program's name refers to its modular structure which facilitates the insertion of new subroutine packages to handle specific tasks. The version used here, MODFLOW/mt, was obtained from Dr. Chunmiao Zheng, the author of MT3D, and

incorporated several new subroutine packages which are described below. Flexibility, robustness, clarity of coding, and outstanding documentation all contributed to the selection of MODFLOW for this project.

The basic MODFLOW program solves a block centered finite difference approximation to the groundwater flow equation on a variable cell size, three dimensional rectangular grid. MODFLOW allows for anisotropy so long as the grid axes are aligned with the principal directions of hydraulic conductivity. It can solve either steady or transient cases and provides options for recharge, wells, and other hydrologic features. Both confined and unconfined aquifers can be modeled. The original block centered flow package (BCF1) allowed the dewatering of layers during periods of water table decline, but could not handle rewetting due to a rising water table. This was an important limitation in modeling MADE-2 due to the pronounced water table fluctuations which were observed. The version used here incorporated BCF2 (McDonald, Harbaugh, Orr, and Ackerman; 1991), a newer package which allows rewetting. The present MODFLOW also incorporated PCG2 (Hill, 1990), a preconditioned conjugate gradient solver; LKMT18, which generates output files in a format suitable for input to MT3D; and STR1, a stream interaction package which was not used.

The user of MODFLOW must input the grid geometry, boundary and initial conditions, values related to the principal hydraulic conductivities for each cell, storage coefficients for each cell, and source parameters.

The definition of a suitable computational grid is the first step in applying MODFLOW. In view of the heterogeneity of the site and the nature of the plume, a uniform three dimensional grid was selected. As in Gray (1993), the grid consists of 9 layers, each containing 66 rows and 21 columns of 5 m x 5 m cells. The horizontal grid is identical to that of Gray (1993) with the 105 m and 330 m sides parallel to the x and y axes of the MADE-2 coordinate system, respectively. The origin of the MADE-2 coordinate system is at the center of the cell which contains all 5 injection wells (row 61, column 11). In terms of MADE-2 coordinates, the domain extends from -52.5 m to +52.5 m in the x direction and from -27.5 m to +302.5 m in the y direction.

One of the most critical steps in the development of a numerical model is geostatistical analysis, the process by which a relatively small number of irregularly spaced observations of some variable are used to assign values at the relatively large number of regularly spaced computational nodes. Gray (1993) used the commercial program SURFER for this task. In the present study the public domain software package Geo-EAS Version 1.2.1 (Englund and Sparks, 1991)

was employed. Geo-EAS is a menu driven personal computer program developed by the Environmental Protection Agency (EPA) primarily to perform two dimensional kriging. Geo-EAS allows the user to closely control most aspects of the kriging process, including the selection of linear, spherical, exponential, or Gaussian variograms. The program can also calculate descriptive statistics and produce two dimensional contour plots. In comparison with SURFER Version 4, Geo-EAS is less polished, has inferior graphics, and has more glitches, e.g. the Gaussian variogram doesn't always work. On the other hand, Geo-EAS is more flexible and is much less of a black box. In this study all kriging was done using Geo-EAS, but most of the final contour plots were made using SURFER Version 4.

Geological logs from 32 locations scattered over and near the site were analyzed to determine the vertical boundaries of the aquifer. Program XLTOGE was written to reformat the measured ground surface and aquitard top elevations for input to Geo-EAS. These data were kriged using a linear variogram for the ground surface elevation and a spherical variogram for the aquifer bottom elevation. The ground surface elevation was estimated to vary from 64.68 m to 65.99 m, and the aquifer bottom was estimated to range from 49.90 m to 55.51 m MSL.

The rewetting capability of the BCF2 package allowed for a more efficient vertical grid spacing that had been used previously. In Gray (1993), the computational domain was bounded below by an impermeable plane at 51.0 m, and the lower 8 layers were each 1 m thick. The top layer, with a base at 59.0 m, had an upper boundary which fluctuated with the water table. As the observed water table reached its peak in May 1991, cells in the top layer were up to 6.1 m thick. This was undesirable from the standpoint of accuracy, but was necessary because BCF1 required the lower boundary of the top layer to be low enough to guarantee against dewatering.

In the present grid the base of the upper layer is at 63.0 m, so that its saturated thickness should never exceed 2.1 m. The next seven layers are each 1 m thick. The top of the lowest layer is at 56.0 m, and its impermeable bottom varies to match the top of the aquitard. The thickness of the lowest layer ranges from 0.49 m to 6.10 m with a mean of 3.31 m. In terms of MODFLOW classification, layer 1 is unconfined, layers 2 through 7 are fully convertible (LAYCON = 3), and layers 8 and 9 are confined.

There were 82 piezometers scattered irregularly over and near the computational domain. Heads were recorded continuously in 16 piezometers. There were also 17 manual piezometer surveys conducted at intervals of about one month and typically covering 45 piezometers. The continuous and survey observations showed good

agreement. From the first observations, about 1 week before injection, until about 180 days after injection, heads declined smoothly less than 1 m. After that date heads underwent larger and more erratic changes. These results showed that a transient model was essential.

The piezometric heads from the monthly surveys were needed to establish the initial head at each node, as well as the head at each boundary node as a function of time. Using SURFER, Gray (1993) kriged using all of the available heads, pooling all depths and including piezometers which were far from the computational domain. The results were assigned as initial and boundary conditions to all layers, i.e. there was no variation of head with depth. The numerical solutions obtained with these conditions showed heads which dropped toward the northwest corner of the grid, suggesting that the plume should bend toward the northwest. As the observations showed the plume bending toward the northeast, it was important to be more careful in translating the observed heads into initial and boundary conditions.

The commercial spreadsheet Quattro Pro for Windows was used to examine the distribution of the piezometer screen midpoint elevations. It was noticed that most were close to either 60.5 m or 56.0 m. Geo-EAS was used to reject piezometers which were not close to these elevations or were too far outside the computational domain. The pizometers selected for kriging consisted of an upper set of 15 whose screen midpoints ranged from 59.76 m to 61.22 m with a mean of 60.55 m, and a lower set of 23 whose elevations were between 55.51 m and 56.71 m with a mean of 55.95 m. Figure 1 shows that the coverage of the (plan) north end of the computational domain was sparse at both levels.

MADETOGE was written to segregate the monthly piezometer survey data into upper and lower piezometer files. These files were kriged with linear variograms using Geo-EAS. Figure 2 shows the results for the upper and lower piezometer sets for the survey of March 8, 1991. In almost every survey the heads at both levels decline toward the northwest. The upper level heads were assigned to layers 1 through 4, and the lower level heads to layers 8 and 9. Heads were specified for layers 5, 6, and 7 by linear interpolation. Program BASMAKER wrote the MODFLOW Basic package input file which included the initial heads at every node. Program GHBMAKER created the input file for the MODFLOW General Head Boundary package. The function of this package was to maintain specified heads at every boundary node (Dirichlet boundary conditions).

The net recharge was the difference between precipitation and evapotranspiration. Daily precipitation and temperature data were measured at

the CAFB weather station, less than 2 km from the test site. Daily pan evaporation data from State University, about 35 km distant, were supplied by State Climatologist Dr. C. L. Wax. Missing evaporation data were estimated from the daily maximum temperatures using the empirical equation of Pote and Wax (1986). Based on the recommendation of Dr. Wax, a pan coefficient of 0.8 was used to estimate the evapotranspiration.

The 17 piezometer surveys and the two day injection period were used to define 18 stress periods during which all boundary conditions and water sources were constant. These were the same periods used by Gray (1993). Except for the injection period, the stress periods were approximately centered on the survey dates. The recharge rates were the averages of the daily values. Table 1 defines the stress periods used in MODFLOW. The injection occurred at a rate of 4.85 m^3/day on simulation days 15 and 16 at row 61, column 11, and layer 7. A constant time step of 2 days was used in all the MODFLOW simulations.

Table 1. Stress periods and recharge rates used in MADE-2 simulations.

stress period	starting date	starting sim. day number	period length [days]	head survey date	survey sim. day number	recharge rate [m/day]
1	June 12	1	14	June 19	8	-0.00313
2 *	June 26	15	2	"	"	-0.00478
3	June 28	17	36	July 23	42	-0.00148
4	Aug. 3	53	28	Aug. 13	63	-0.00409
5	Aug. 31	81	32	Sept. 17	98	-0.00286
6	Oct. 2	113	26	Oct. 15	126	-0.00107
7	Oct. 28	139	24	Nov. 7	149	+0.00071
8	Nov. 21	163	32	Dec. 5	177	+0.00942
9	Dec. 23	195	32	Jan. 8	211	+0.00387
10	Jan. 24	227	30	Feb. 8	242	+0.00809
11	Feb. 23	257	28	Mar. 8	270	+0.00114
12	Mar. 23	285	30	Apr. 4	297	+0.00794
13	Apr. 22	315	24	May 10	333	+0.01022
14	May 16	339	18	May 20	343	+0.00357
15	June 3	357	24	June 13	367	+0.00046
16	June 27	381	34	July 9	393	-0.00273
17	July 31	415	32	Aug. 19	434	-0.00159
18	Sept. 1	447	22	Sept. 11	457	-0.00384
last day	Sept. 22	468				

* injection period

Vertical profiles of horizontal hydraulic conductivity were measured in 67 wells scattered in and around the computational domain. The data were measured over successive 15 cm layers using a borehole flowmeter. The gaps where the well screens were jointed were filled in with the values immediately above and below. The height profiled and the layer boundaries varied from well to well.

KAVG94 was written to relate these profiles to the grid layers. The tops of the profiles varied from 57.62 m to 62.68 m. The program extended each profile up to 64.0 m using the conductivity at the top of the profile. The lowest points varied from 51.88 m to 56.22 m. Profiles were extended down to 56.0 m or the next lower integer elevation using the conductivity at the lowest point. The extended profiles were averaged arithmetically over each MODFLOW layer to generate horizontal conductivities. With the assumption that each 15 cm slice of material was isotropic, the extended profiles were averaged harmonically between the midpoints of the MODFLOW layers to generate vertical leakances. Leakance is the vertical conductivity divided by the thickness between adjacent nodes. Due to the variable thickness of layer 9, the leakance between layers 8 and 9 was calculated for the interval from 56.5 m to 55.5 m rather than to the actual midpoint of the lowest cells. Exceptions occurred at wells K-2, K-26, and K-28 where the profiles ended at 56.0 m.

The next task was to interpolate and extrapolate the averaged profiles horizontally so as to obtain the horizontal conductivity and vertical leakance at each node of the computational grid. The averaged profiles were log transformed using KA2LOG, kriged with Geo-EAS, and transformed back by DLOGFILE. The log transformation was necessary to avoid negative values in the kriging process. Spherical or exponential variograms were used. Program BCF2MAKER was written to format the conductivity values for input to the MODFLOW BCF2 package.

During execution, MODFLOW calculates the transmissivity of the cells which are partially saturated by multiplying the horizontal conductivity of the cell by its saturated depth. Since the horizontal hydraulic conductivity represents an average over the entire cell thickness, this is correct only if the cell is truly homogeneous. The vertical leakance is treated as a constant as long as a cell contains water, even though it represents an average over the full region between nodes. This is not correct either.

Little was known about the storage coefficients. A specific yield of 0.1 was measured in a single traditional pump test (AT-2) (Boggs, Young, Benton, and Chung; 1990). No measurements of specific storage were made, so a confined

storage coefficient base value of 0.0001 was assumed, based on textbook values for specific storage in sand and sandy gravel (Anderson and Woessner, 1992). In view of the great uncertainty of these parameters, simulations were run with higher and lower values in order to investigate the sensitivity of the results. In each simulation, the storage coefficients were constant throughout the grid. In reality, great variability is expected; but there was no defensible way to account for this on the basis of the available data.

The 468 day experiment was simulated on a Sun Sparcstation 2 using the PCG2 solver. In spite of the rather severe vertical motion of the water table, MODFLOW performed reliably. Table 2 lists the differences among the five cases which were computed.

Table 2. MODFLOW simulation summary.

Case	RELAX	WETDRY [meters]	specific yield	confined storage coef.	run time [min.]	final volume error
1	0.98	-0.1	0.1	0.0001	60	-0.25%
2	1.00	-0.1	0.1	0.0001	unknown	-0.24%
3	0.98	-0.01	0.1	0.0001	72	-0.25%
4	0.98	-0.1	0.2	0.0005	94	-1.52%
5	0.98	-0.1	0.05	0.00005	58	-0.23%

Taking Case 1 as the base case, Case 2 tests the effect of increasing RELAX, a convergence parameter in the PCG2 solver package. This variation left the solution virtually unchanged. Case 3 examines the effect of reducing WETDRY, a parameter in the BCF2 package which controls cell rewetting. The negative sign indicates that the rewetting of cell x depends on the head in the cell below. The absolute value of WETDRY is the amount by which the head in the cell below must exceed the bottom elevation of cell x before it rewets. Case 3 results were virtually identical with Case 1. A positive value of WETDRY makes rewetting depend on the heads in the four horizontally adjacent cells. Runs with positive values of WETDRY invariably failed to converge.

Cases 4 and 5 varied the storage coefficient values. It can be seen that increasing the storage coefficients increases the volumetric discrepancy and the run time. The effects on the nature of the solution are discussed further below, but they have not yet been fully assessed.

Figure 3 presents the Case 1 head contours on simulation day 270 (March 8, 1991) in layers 4 and 9. Compared with the kriged distributions for the upper and lower piezometers on the same day shown in Figure 2, it can be seen that the head distributions are both qualitatively and quantitatively similar. In both the

predicted and observed cases, the flow is downward. The tendency for the heads to decline toward the northwest is evident in this figure and throughout the simulation.

In order to obtain a numerical measure of agreement, the simulated heads were compared to the continuous head observations. Program WELLGRPH was written to extract from the MODFLOW binary output file the head time series for those cells which contained continuously monitored piezometers. The continuous piezometer records show erratic day to day variations which cannot be predicted by a model whose boundary conditions change only 16 times in 468 days. To provide a reasonable basis of comparison, the daily observed heads were averaged over each stress period by program HYDROGRA. Figure 4 compares the Case 1 predictions to the observed (averaged) heads at two piezometers with the same horizontal position. The simulated results adjust rapidly to the boundary conditions for each stress period. The model results are better at the upper level (P55a) than at the lower level (P55b), where the model overpredicts markedly in stress periods 9, 11, and 13.

The averaged observations were subtracted from the unaveraged MODFLOW heads and the maximum, minimum, and root mean square (rms) differences were summarized in Table 3. Case 5, with the smallest storage coefficients, gives the best overall accuracy. Case 4 has the greatest excursions from the observations, yet its rms deviation is smaller than Case 1. Although the ability of the model to reproduce the observations is imperfect, it is hard to see how the model could be improved given the limitations of the data base.

Table 3. Deviation of MODFLOW heads from continuous observations [meters].

	min.	min.	min.	max.	max.	max.	rms	rms	rms
Well	Case 1	Case 4	Case 5	Case 1	Case 4	Case 5	Case 1	Case 4	Case 5
P53a	-0.65	-1.32	-0.57	0.74	0.51	0.14	0.329	0.228	0.194
P54a	-0.53	-0.84	-0.37	0.39	0.58	0.30	0.143	0.165	0.136
P54b	-0.42	-0.78	-0.17	0.43	0.52	0.43	0.147	0.159	0.143
P55a	-0.53	-0.80	-0.37	0.44	0.50	0.44	0.199	0.204	0.199
P55b	-0.12	-0.44	+0.01	1.01	1.01	1.01	0.374	0.374	0.374
P60a	-0.51	-0.51	-1.51	0.30	0.38	0.30	0.188	0.188	0.188
P61a	-0.40	-0.40	-0.40	0.36	0.36	0.36	0.188	0.188	0.188
P61b	-0.39	-0.39	-0.39	0.23	0.23	0.23	0.154	0.154	0.154
average	-0.44	-0.69	-0.35	0.49	0.51	0.40	0.215	0.208	0.197

TRANSPORT MODELING

MT3D is a public domain program developed for the EPA to solve the three dimensional groundwater transport equation for dissolved contaminants (Zheng, 1990). MT3D is coded in Fortran 77 and uses the same modular structure as MODFLOW. In fact, MT3D accepts as input the head and flux distributions computed by MODFLOW (or similar flow models). MT3D then predicts the concentration field of a single contaminant which undergoes advection, dispersion, and chemical reactions. The program provides for various types of point and area sources and sinks including wells, recharge, and flows through the domain boundaries. MT3D Version 1.80 was used in this study.

Because of the computational difficulties of numerical dispersion and oscillation in advection-dominated flows, MT3D incorporates four options for calculating the advection term. The Method of Characteristics (MOC) tracks a large number of imaginary tracer particles forward in time. The Modified Method of Characteristics (MMOC) tracks particles located at the cell nodes backward in time. The MMOC requires much less computation than the MOC, but it is not as effective in eliminating artificial dispersion, especially near sharp fronts. The Hybrid Method of Characteristics (HMOC) uses the MOC near sharp concentration gradients and the MMOC in the remainder of the domain. An Eulerian Upstream Differencing (UD) option is provided for problems in which advection does not dominate.

The dispersion terms are computed using a fully explicit Eulerian central difference method. For isotropic media, the dispersion coefficients are based on longitudinal and transverse dispersivities. For more complex situations, there is an option which distinguishes horizontal and vertical transverse dispersivities. The explicit formulation reduces the memory needed, but requires limits on the time step to assure numerical stability. Consequently each flow model time step may be automatically subdivided into several transport steps in order to maintain numerical stability in MT3D.

MT3D allows both equilibrium sorption and first order irreversible rate reactions. Equilibrium sorption reactions transfer contaminant between the dissolved phase and the solid phase (which is sorbed to the soil matrix) at time scales much shorter than those of the flow. These reactions may be described by linear isotherms or nonlinear isotherms of the Freundlich or Langmuir types. In first order irreversible rate reactions the rate of mass loss is linearly proportional to the mass present. This class includes radioactive decay and

certain types of biodegradation.

MT3D requires information beyond that needed for and calculated by MODFLOW. A porosity is needed for each cell in order to calculate seepage velocities, yet porosities were measured in only four core holes. The 84 samples had a mean porosity of 0.32, and this value was used for every cell. Based on the MADE-2 observations and an assumed two dimensional analytical model for the plume, Boggs and others (1993b) estimated the longitudinal dispersivity to be 10 m and the transverse horizontal dispersivity to be less than 2.2 m. The base values of dispersivity used were 10 m in the longitudinal direction, 1 m in the horizontal transverse direction, and 0.1 m in the vertical transverse direction. For the purpose of calculating concentrations, every wetted layer was assumed to have a uniform thickness of 1 m, although the actual thickness varied for the top and bottom layers.

MT3D was applied only to the tritium plume. The molecular diffusion coefficient of tritium in water, calculated using the Wilke-Chang method, was multiplied by an assumed tortuosity of 0.25 to yield the value of 2.16×10^{-4} m^2/day for the molecular diffusion coefficient of tritium in a saturated porous medium. The injected fluid had a tritium concentration of 0.0555 Ci/m^3; and the natural background, including recharge and boundary inflows, was set to zero. Water leaving the domain carried the concentration of the cell it last occupied. Sorption does not affect tritiated water, but tritium decays with a 12.26 year half-life.

The transport simulations attempted, all based on the Case 1 MODFLOW head solution, are summarized in Table 4. None are remotely satisfactory. No run extended beyond simulation day 141 because by that time each had experienced a numerical failure or had been terminated because the solution was unreasonable. In general, the run times were inconveniently long. The mass discrepancies appear either unacceptably large (MOC, MMOC, and HMOC) or remarkably tiny (UD), but the meaning of this parameter is not clear. Runs 7 (HMOC) and 8 (UD) predicted nearly identical plumes even though the mass discrepancies were very different.

Run 3 produced a widely spread plume even though the dispersion package was turned off. This appears to be a numerical shortcoming of the MMOC method because no-dispersion runs 5 (MOC) and 6 (HMOC) predicted unrealistically small spreads. All of the no-dispersion runs were free from negative concentrations. Run 11 was a repetition of Run 9 using double precision arithmetic; the results were identical. In Runs 9 and 11 the dispersivities in the longitudinal,

transverse horizontal, and transverse vertical directions were 4.0 m, 0.4 m, and 0.4 m, respectively. Runs 12 (UD) and 14 (HMOC) used dispersivities in the longitudinal, transverse horizontal, and transverse vertical directions of 1.0 m, 0.1 m, and 0.1 m, respectively. In Run 13 (UD) the dispersivities were all 0, but molecular diffusion was active. In general, the smaller the dispersivities, the more realistic the plume appeared.

Table 4. Summary of MT3D simulations.

Run	advection method	dispersion	long. dispersivity [m]	last sim. day	run time [hours]	mass discrep.	plume characteristics
1	HMOC	yes	10.0	30.2*	15.75	+7.93%	wide spread, some < 0
2	MMOC	yes	10.0	5.0*	1.75	n.a.	injection not started
3	MMOC	no	n.a.	129.4	10.4	+82%	wide spread
4	HMOC	no	n.a.	20.4*	0.72	+19.2%	not recorded
5	MOC	no	n.a.	62.1*	3.5	-13.1%	confined to 7 cells
6	HMOC	no	n.a.	140.9	17.38	+17.2%	confined to 8 cells
7	HMOC	yes	10.0	44.6*	47.05	+4.55%	wide spread lots < 0
8	UD	yes	10.0	61.2	16.6	-0.0001%	wide spread, lots < 0
9	UD	yes	4.0	90.4	<21.4	+0.0001%	wide spread, lots < 0
11	UD **	yes	4.0	90.4	<29	+0.0001%	identical to case 9
12	UD	yes	1.0	128	<5.37	+0.0002%	realistic, lots <0
13	UD	yes	0.0	138.3	<8	+0.0003%	realistic, few <0
14	HMOC	yes	1.0	105.9*	<12.6	+12.3%	realistic, lots <0

* run terminated by user. ** double precision.

CONCLUSIONS

1. Geo-EAS Version 1.2.1 is technically superior to SURFER Version 4. It provides a satisfactory tool for exploratory data analysis and two dimensional kriging. SURFER has better graphic capabilities.

2. Three dimensional groundwater flow simulations using MODFLOW are practical and consistent. The rewetting capability of the BCF2 package improves the accuracy of simulations in which the water table fluctuates as much as in MADE-2.

3. Although the flow model has not been subjected to grid refinement or extensive parametric variation studies, the comparison between the simulated and observed heads is satisfactory. Given the existing data, there is little prospect for significant improvement.

4. The simulated head distribution suggests that the plume should bend toward the northwest. The observations show the plume bending toward the northeast. This discrepancy is probably due to inaccurate head boundary conditions caused by a lack of piezometers near the northern end of the grid.

5. We were unsuccessful in our attempts to simulate the spread of the tritium plume using MT3D. Further efforts to achieve complete, accurate simulations of the tritium plume should be made.

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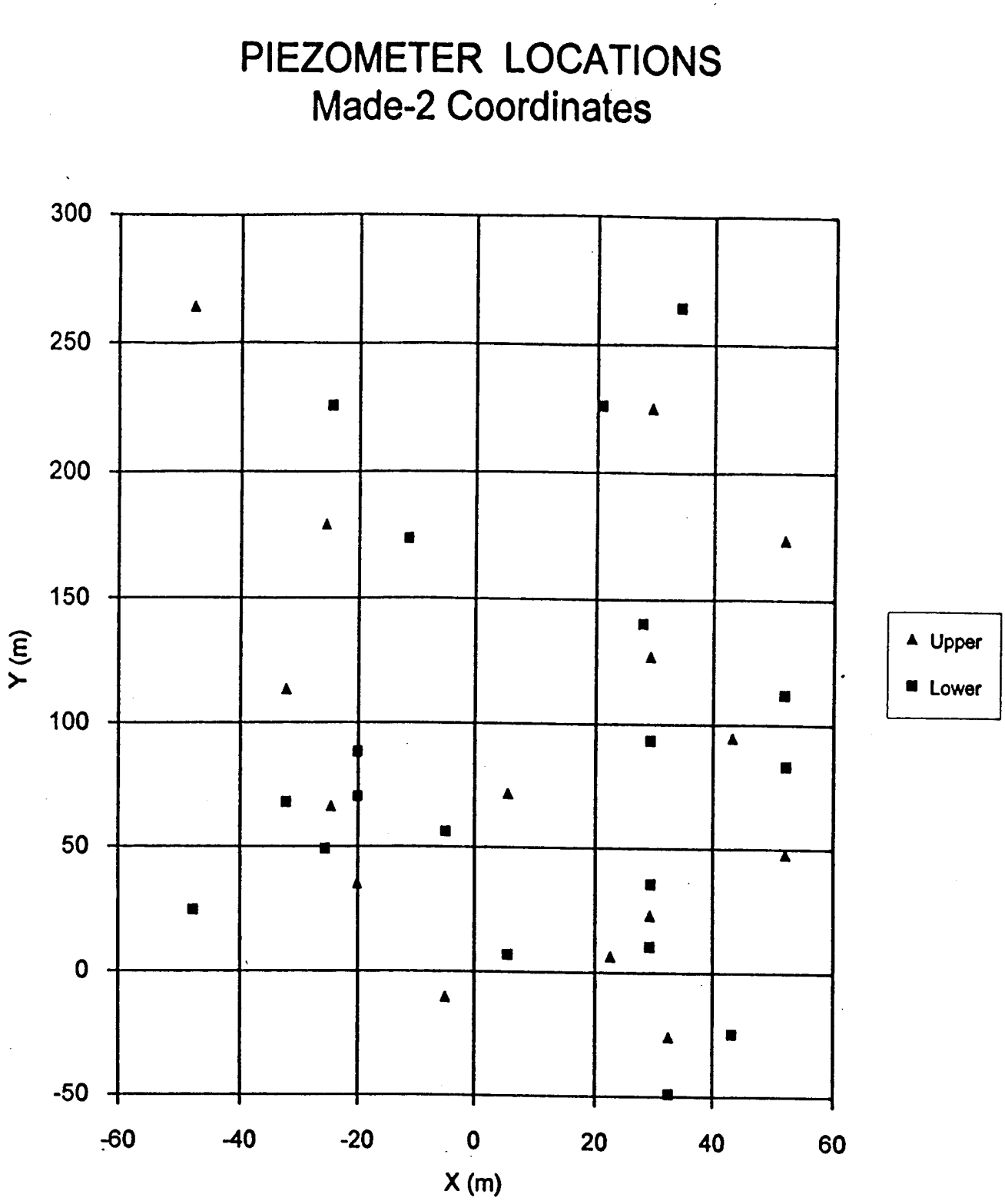

Figure 1. Locations of upper (squares) and lower (triangles) piezometers used to establish initial and boundary conditions. Four locations are common to both sets.

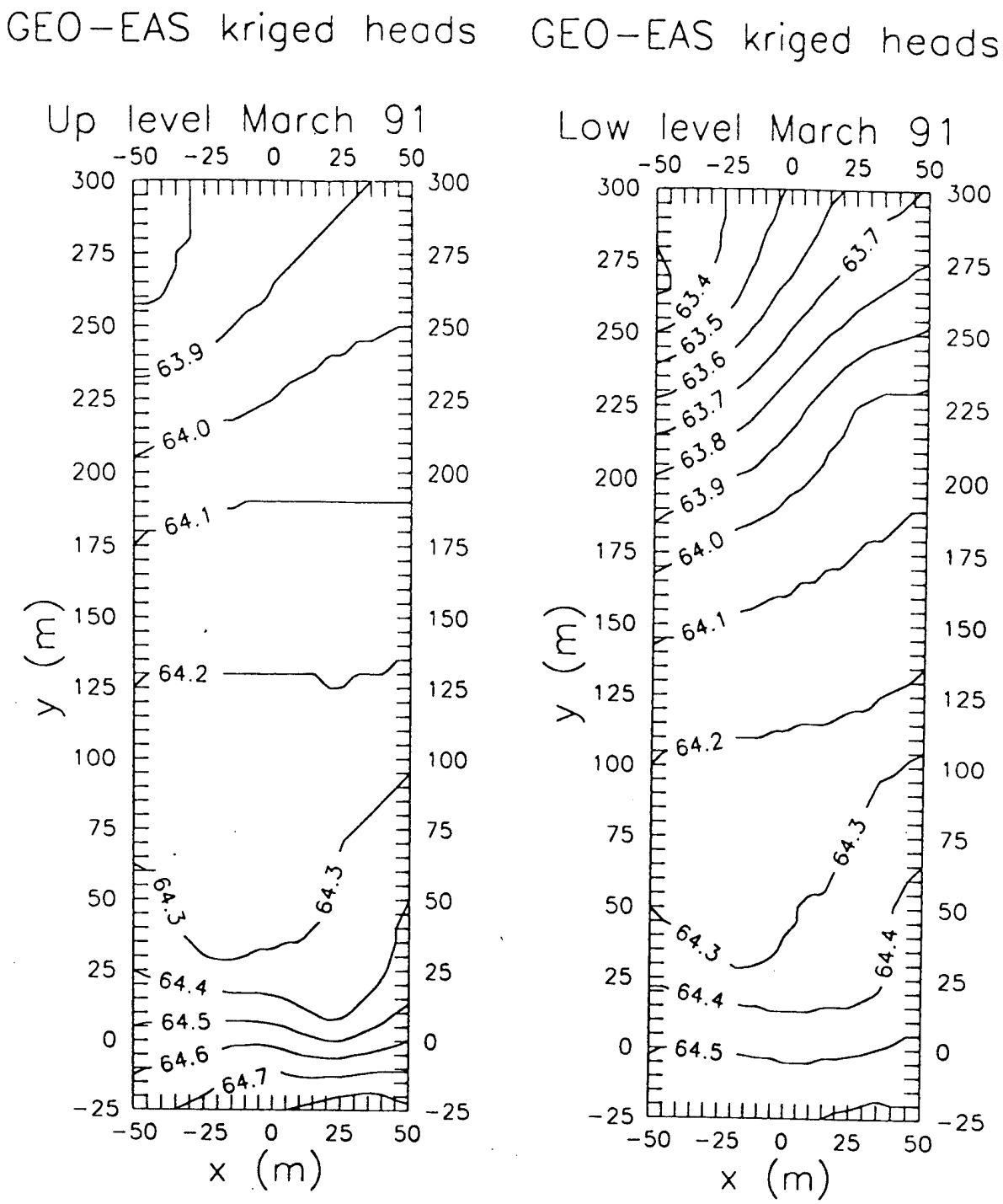

Figure 2. Upper (left) and lower (right) kriged head distributions for simulation day 270 (March 8, 1991). Heads are in meters.

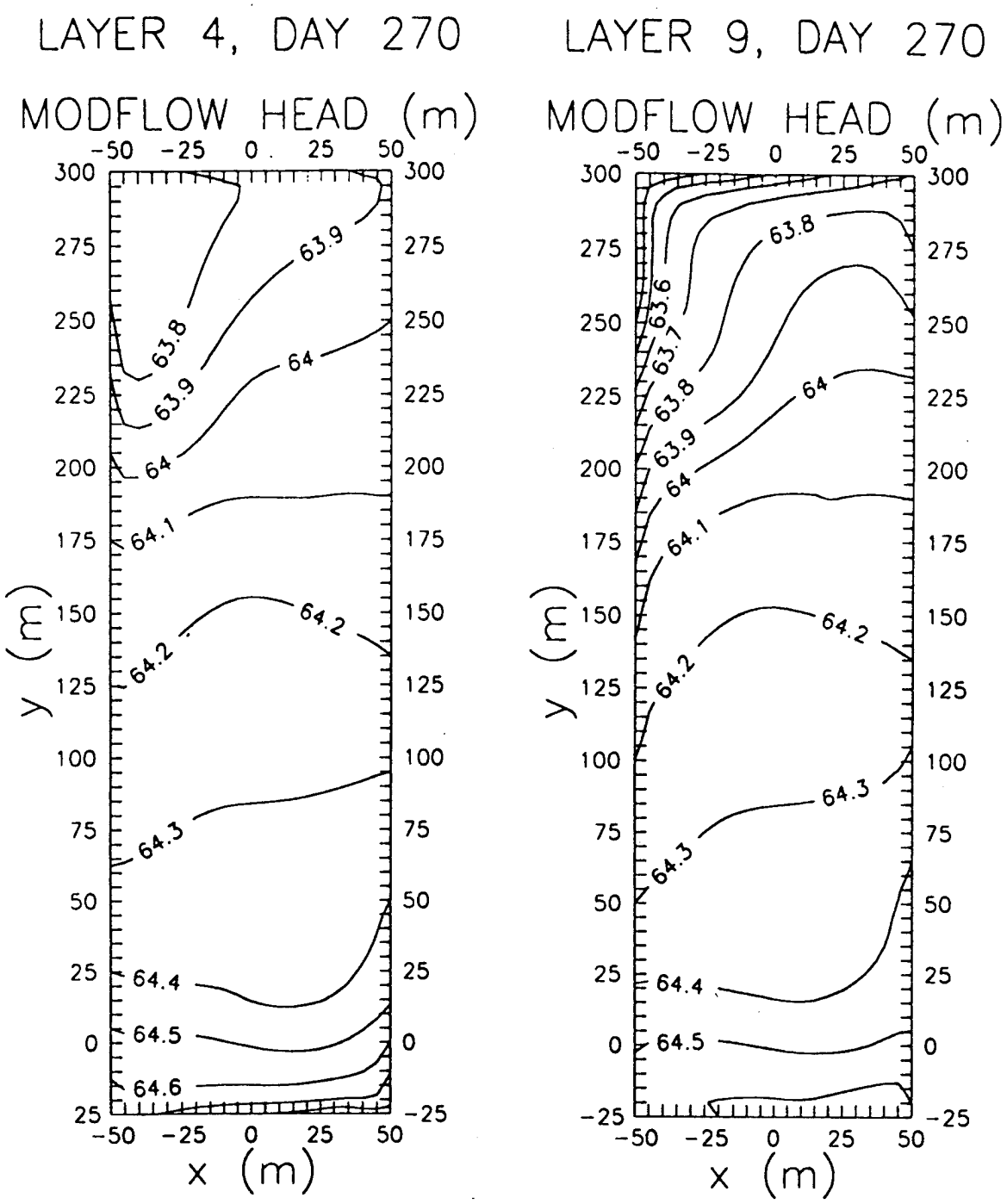

Figure 3. MODFLOW Case 1 simulated heads for layers 4 (left) and 9 (right) for simulation day 270 (March 8, 1991). Heads are in meters.

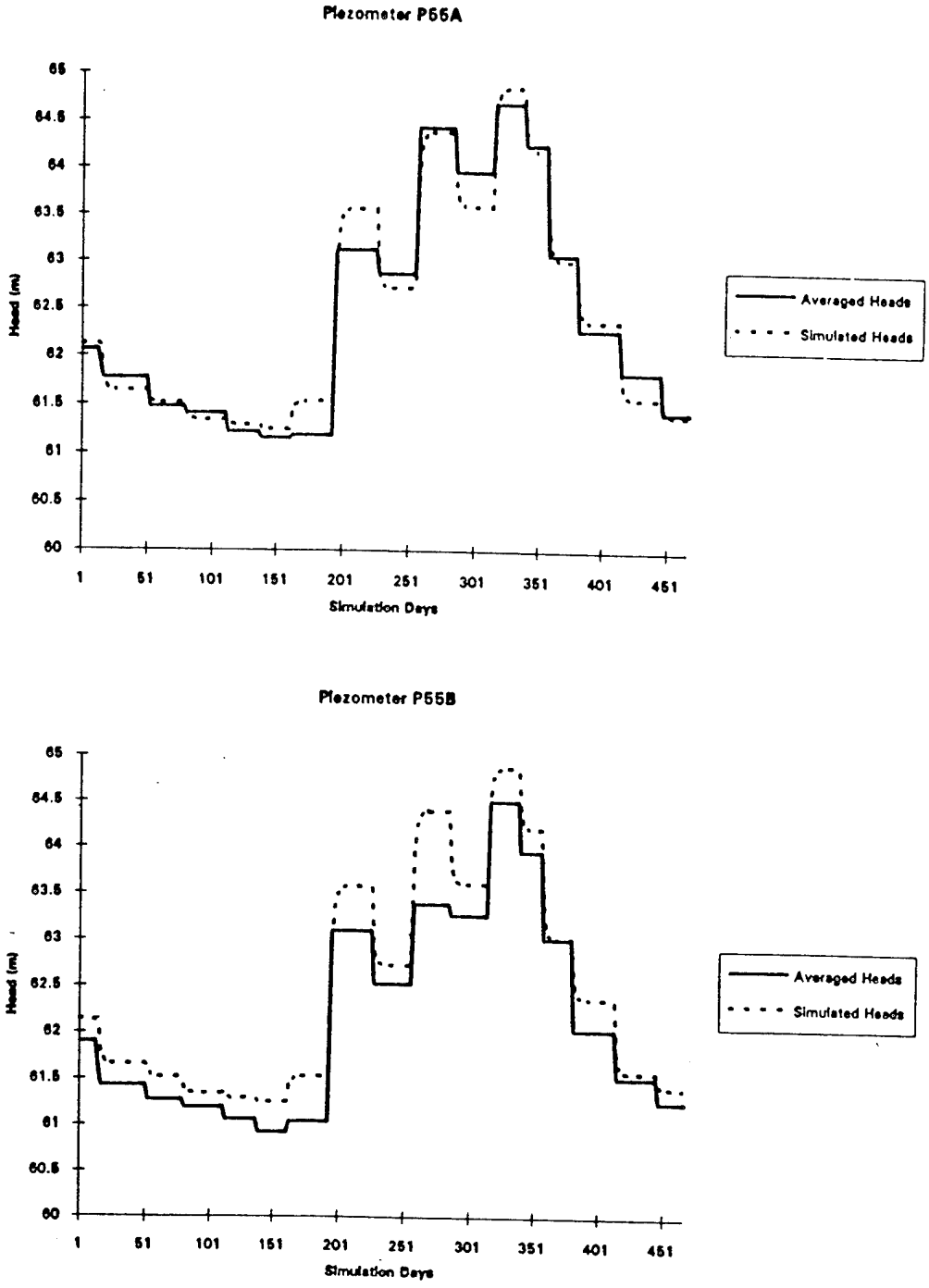

Figure 4. Comparison of MODFLOW Case 1 simulated heads with observed heads averaged over stress periods at piezometers P55a (top) and P55b (bottom). Heads are in meters.